



# WORKSHOP ON TIME DOMAIN SCIENCE USING X-RAY TECHNIQUES

*Workshop Program and  
Charge to Workshop Participants*

*Lin Chen (Argonne National Laboratory)*

*Steve Milton (Argonne National Laboratory)*

*David Reis (University of Michigan)*

*Linda Young (Argonne National Laboratory)*

***Workshop Chairs***

**August 29 – September 1, 2004, The Abbey, Fontana, Lake Geneva Area, WI**



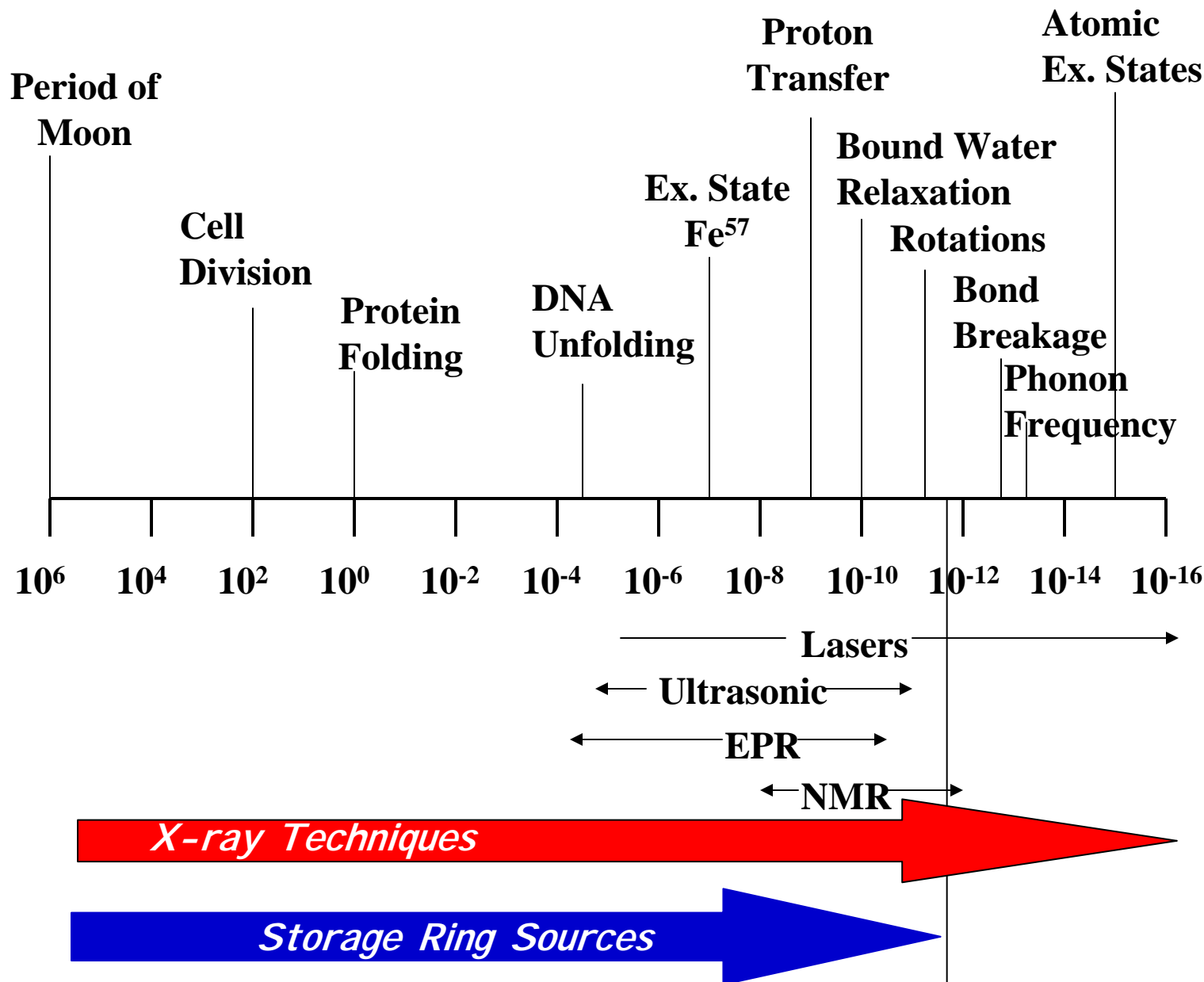
# **Scientific Program Advisory Committee**

- **Philip Anfinrud (National Institutes of Health)**
- **Nora Berrah (Western Michigan University)**
- **Phil Bucksbaum (University of Michigan)**
- **Philip Coppens (SUNY, Buffalo)**
- **Louis DiMauro (Ohio State University)**
- **Stephen Leone (University of California Berkeley)**
- **Gerhard Materlik (Diamond and Chair, APS Science Advisory Committee)**
- **Simon Mochrie (Yale University)**
- **Keith Moffat (University of Chicago)**
- **Jim Norris (University of Chicago and member of APS Science Advisory Committee)**
- **Michael Wulff (ESRF)**

## *Workshop Scope*

- Time domain science is truly multi-disciplinary.
- Advances in time domain science are scientifically and technologically exciting and significant.
- Areas of time domain science where X-ray characterization techniques are potentially useful:
  - Atomic and Molecular Science
  - Biological Science
  - Chemical Science
  - Condensed Matter and Materials Science
- Work at the Third Generation Facilities is an excellent learning pad for launching future experimental programs at the Fourth Generation Facilities

# Scope of Time Domain Considered in this Workshop



August 29 – September 1, 2004, The Abbey, Fontana, Lake Geneva Area, WI

*Challenges*

**Grand Challenges  
In  
Time Domain Science and  
Opportunities for X-ray Techniques  
to Address them**

*Scientific Challenges*

**Gas Phase Dynamics:**

- strong-field control of inner-shell processes
- coherent control of molecular processes
- geometry-dependent photoionization dynamics

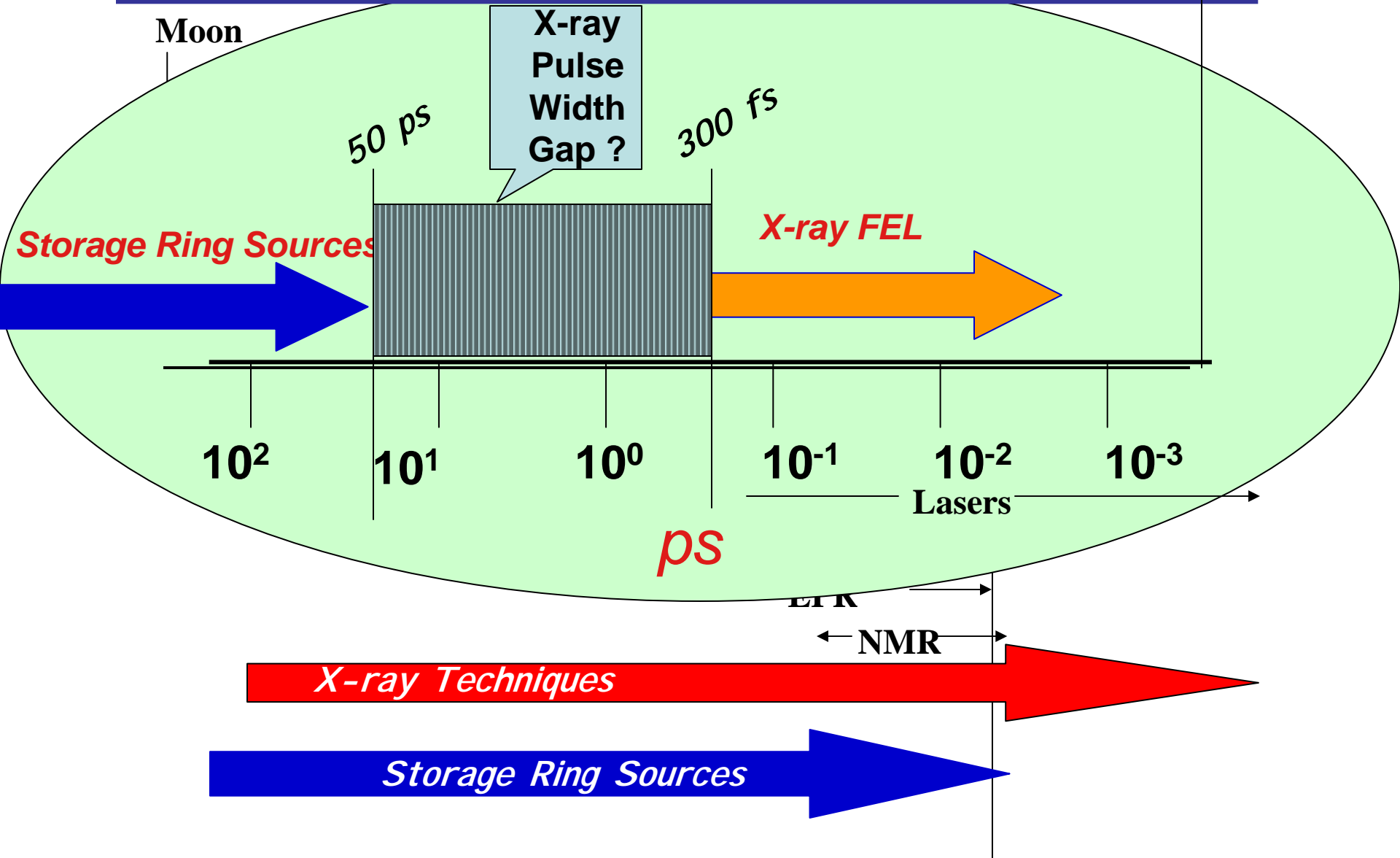
**Chemical and Biological Dynamics:**

- structural dynamics in photochemical reactions of molecules, self-assembled supermolecules, and nanoparticles;
- protein/DNA folding, structural relaxation and enzymatic intermediates;
- structural dynamics of single protein/DNA/nanoparticles;
- coherent structural dynamics in chemical reactions

**Dynamics in Condensed Matter:**

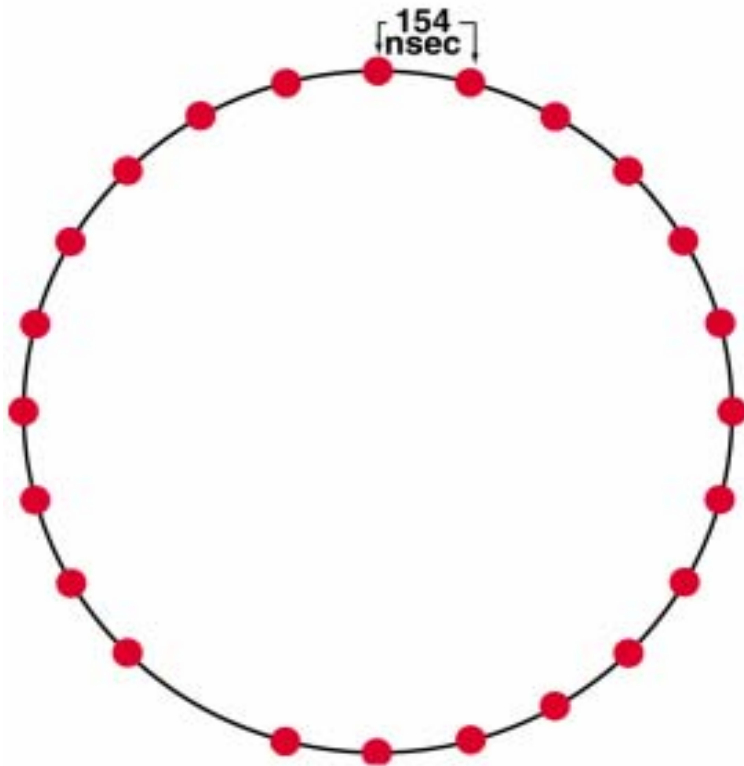
- nonequilibrium electron and phonon dynamics
- phase transitions and domain reversals
- nucleation, growth and phase separation

# *A Challenge to Accelerator Physicists*

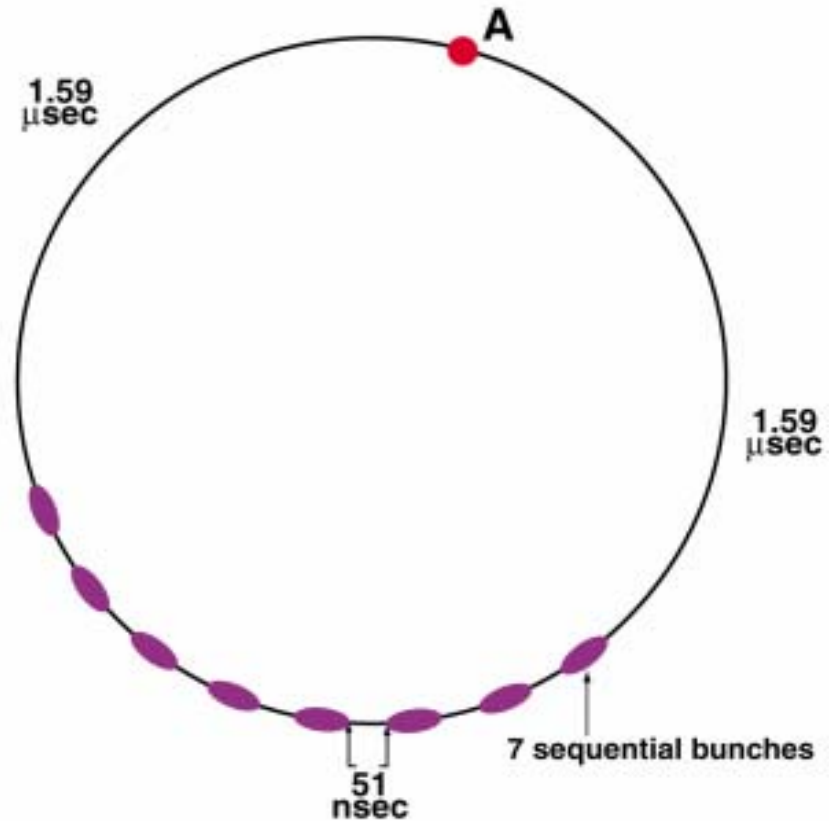


# *Typical Bunch Filling Patterns at APS*

**Singlet 23 Bunches**  
**Normal Fill Pattern**



**Asymmetric (Hybrid) 1 or 3 +  $8 \times 7$**   
**Special Operating Mode**

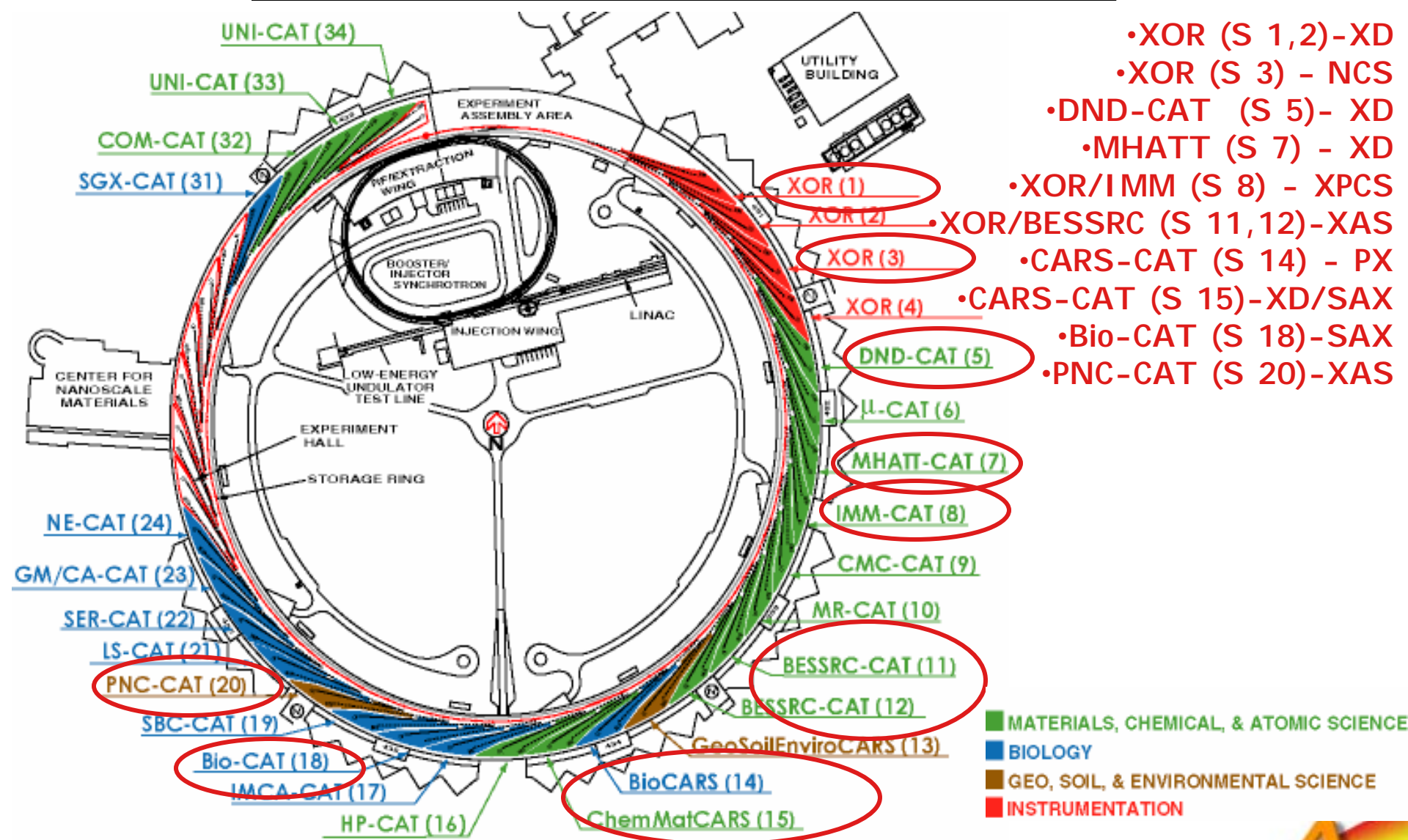




## *Practical Challenges*

- *Higher Beam Brilliance*
  - *Sub-Microsecond Small Angle Scattering (SAX)*
  - *Sub-Microsecond X-ray Photon Correlation Spectroscopy (XPCS)*
- *Higher Current per Single Bunch*
  - *Sub-nanosecond Diffraction*
  - *Sub-nanosecond X-ray Absorption (XAS) and related spectroscopies*
- *Sub-micro to Picosecond Pump-Probe Synchronization*
- *Sub-picosecond Detectors for XD*
- *2-D Low Noise Pixellated Array Detectors for XPCS and SAX*
- *R&D for Time Domain Technique Development*
- *Availability of **in situ** Optical Techniques*

## *APS Time Domain Science Capabilities*



- XOR (S 1,2)-XD
- XOR (S 3) - NCS
- DND-CAT (S 5)- XD
- MHATT (S 7) - XD
- XOR/IMM (S 8) - XPCS
- XOR/BESSRC (S 11,12)-XAS
- CARS-CAT (S 14) - PX
- CARS-CAT (S 15)-XD/SAX
- Bio-CAT (S 18)-SAX
- PNC-CAT (S 20)-XAS

■ MATERIALS, CHEMICAL, & ATOMIC SCIENCE  
 ■ BIOLOGY  
 ■ GEO, SOIL, & ENVIRONMENTAL SCIENCE  
 ■ INSTRUMENTATION

*Draft Workshop Objectives*

- 1. Explore the breadth of science covered by the workshop topics, *not* limiting to synchrotron techniques alone.**
- 2. Identify opportunities for continued scientific discovery and impact using the APS during the next 5-10 years in the multi-disciplinary areas of time domain science.**
- 3. Identify new scientific proposals/programs specific to the emerging areas of Time Domain Science that the participants will bring to the APS during next 5 to 10 years. Also evaluate the capital and operational requirements for these proposals/programs.**

*Draft Workshop Objectives*

- 4. In addition to available beamline capabilities at the APS, identify future needs to support research in this area of science and technology.**
- 5. Address accelerator and detector R&D that will enhance the capabilities of the APS time domain science.**
- 6. Address the need and support for theoretical work to strengthen the experimental research.**
- 7. Prepare a summary document for the archival literature to serve as a roadmap for the time domain research using x-rays at the APS Source and suggest the role of the Advanced Photon Source towards this objective.**

## *Charge to the Participants*

1. I identify science and technological problems in the field of time domain science to be addressed during the next 5-10 years using APS
2. I identify and justify the technical requirements to meet the grand challenge problems:
  - New instrumentation and techniques that need be developed on existing beamlines to perform new kind of science.
  - Need for new dedicated beamlines and instrumentations for this community
3. I identify both short- and long-term R&D needs in the accelerator, synchronization, and detector areas that will prepare the community to address grand challenge problems

## *Workshop Report*

- The summaries and slides provided by the speakers of the talks can be accessed directly by clicking the 'summary' or 'slides' in the 'program' on the workshop website.
- You can continually input your thoughts using the 'Swiki' software linked to the lap-top using Wi-Fi Input can be made even after the workshop.

<http://swiki.anlgh.org/Timedomain>

Login Name: time

Password: pico

- Address the applicable objectives in each of the topics in the scope of the workshop after each talk and make recommendations to the APS



# APS Strategic Planning Meeting

**"Future Scientific Directions"** September 2 & 3, Fontana, Wisconsin  
[www.future.aps.anl.gov/Future/Strategic\\_Planning\\_Meeting/home.htm](http://www.future.aps.anl.gov/Future/Strategic_Planning_Meeting/home.htm)

	Thursday Sept. 2, 2004	Friday Sept. 3, 2004
8:00 am	Introduction & Charge	
<b>8:30 am</b>	<b>Report on Time Domain Workshop</b>	Report on <b>Nanomagnetism</b> Workshop
9:30 am	Report on <b>Inelastic Scattering</b> Workshop	Report on <b>Big Magnet</b>
10:00 am	Break	Break
10:30 am	Report on <b>Imaging Techniques</b> Workshop	Report on <b>High-Energy X-rays</b> Workshop
11:30 am	Report on <b>Meso/Nanoscopic</b> Workshop	Report on <b>Biological Crystallography</b> Workshop
12:30 pm	Lunch Break	Lunch Break
2:00 pm	Report on Membrane Science Workshop	Discussion and Wrap-Up
3:00 pm	Report on BES-Funded Sectors Science	
3:30 pm	Break	
4:00 pm	Report on <b>Environmental</b> Workshop	Adjourn
5:00 pm	Report on <b>Soft X-rays</b> Workshop	
6:30 pm	Dinner	

